



Yasuda-Shedlovsky Result

Sample name: **CS000275**
Assay name: **Fast UV psKa**
Assay ID: **11I-09014**
Filename: **E:\T3 DATA\1109\11I-09014_CS000275_Fast UV psKa.t3r**

Experiment start time: **09/09/2011 15:01:18**
Analyst:
Instrument ID: **T311042**

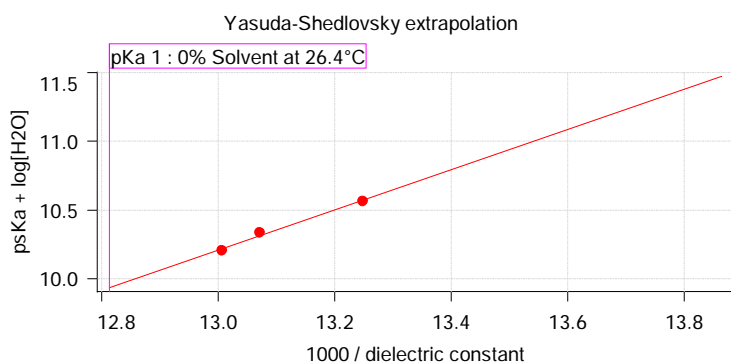
Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R ²	Ionic strength	Temperature
Yasuda-Shedlovsky	8.19	±0.05	-8.82	1463.4649	0.9895	0.211 M	26.4°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H ₂ O]	Ionic strength	Temperature	psKa 1
11I-09014 Points 108 to 161	22.72 %	Up	UV-metric pKa	76.9	43.6 M	0.214 M	26.4°C	✓ 8.56
11I-09014 Points 55 to 107	30.28 %	Up	UV-metric pKa	76.5	39.7 M	0.213 M	26.2°C	✓ 8.73
11I-09014 Points 3 to 54	40.56 %	Up	UV-metric pKa	75.5	34.1 M	0.205 M	26.5°C	✓ 9.03

Graphs

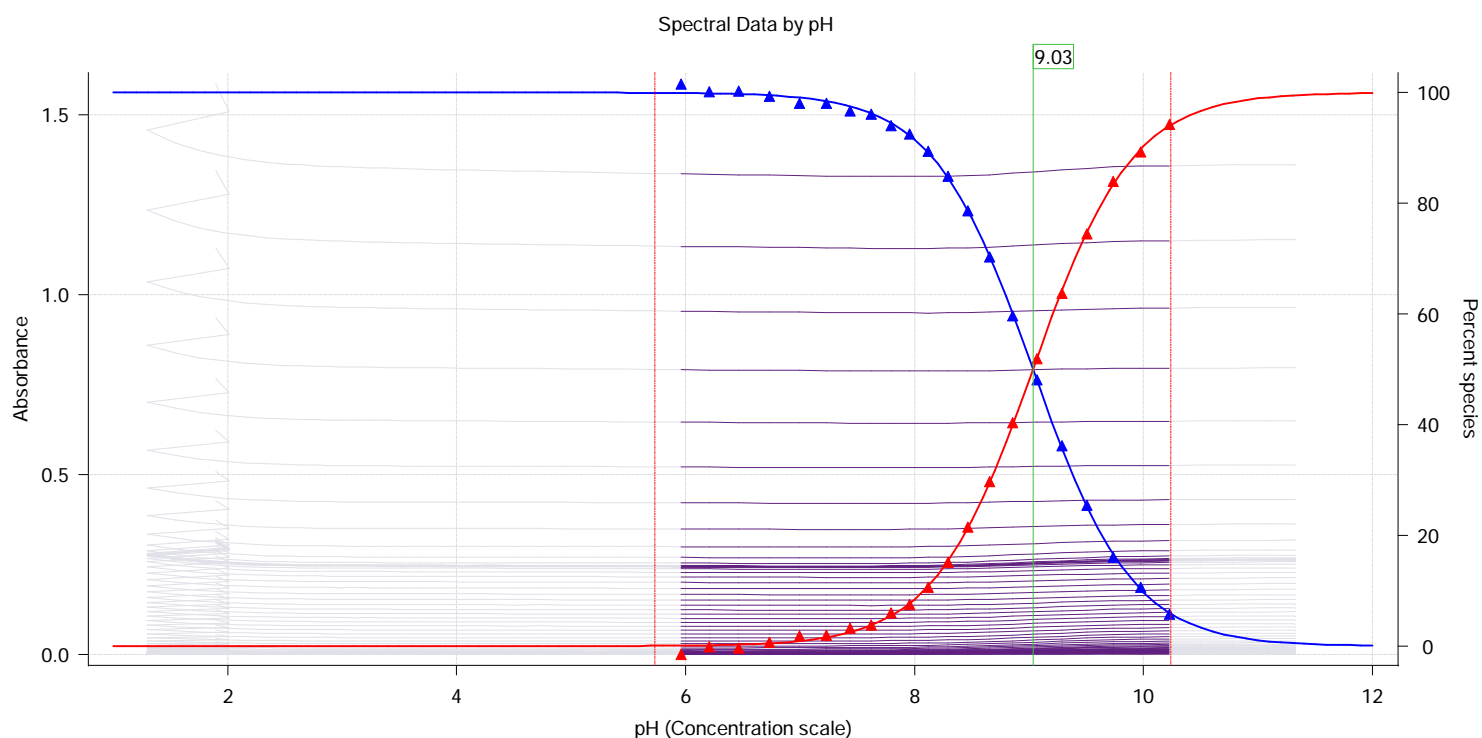
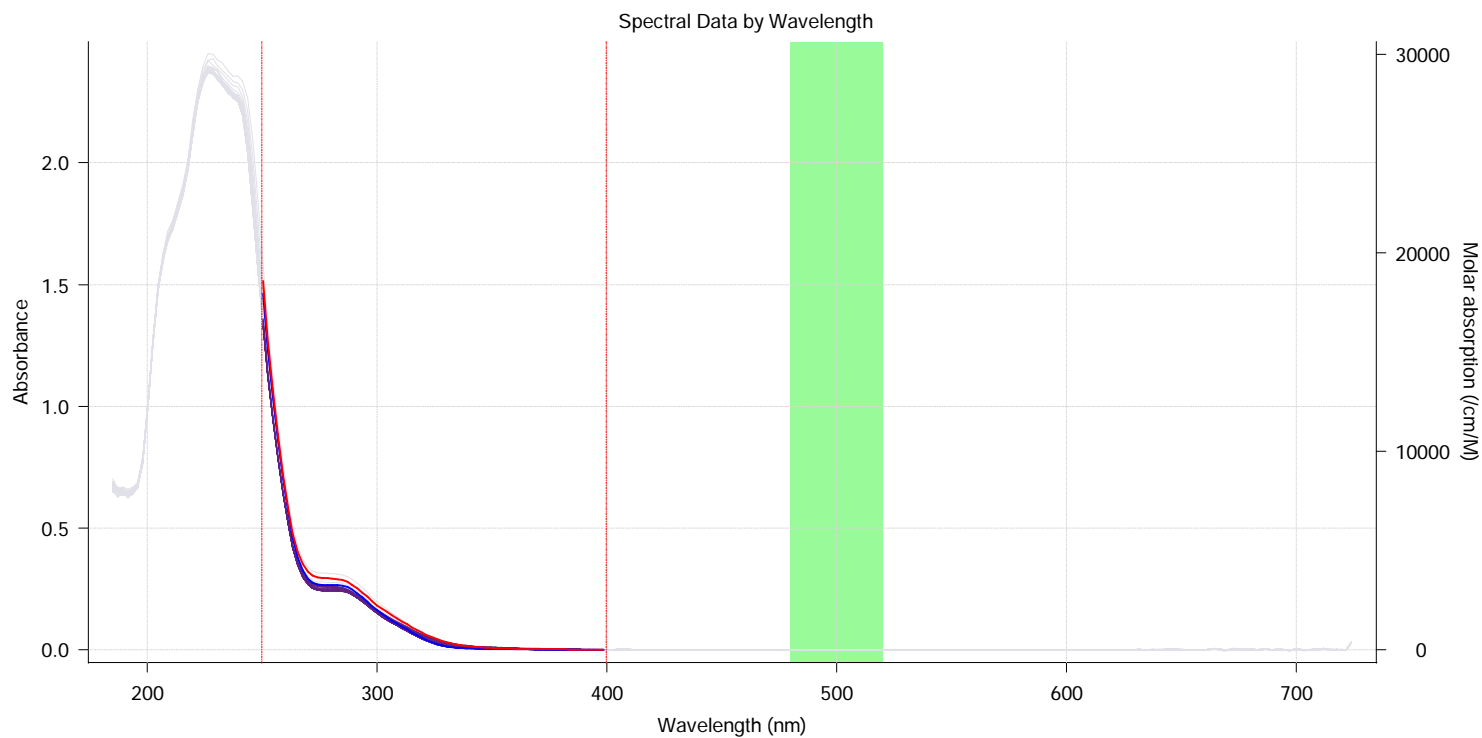


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Fast UV psKa Titration 1 of 3 11I-09014 Points 3 to 54

Graphs

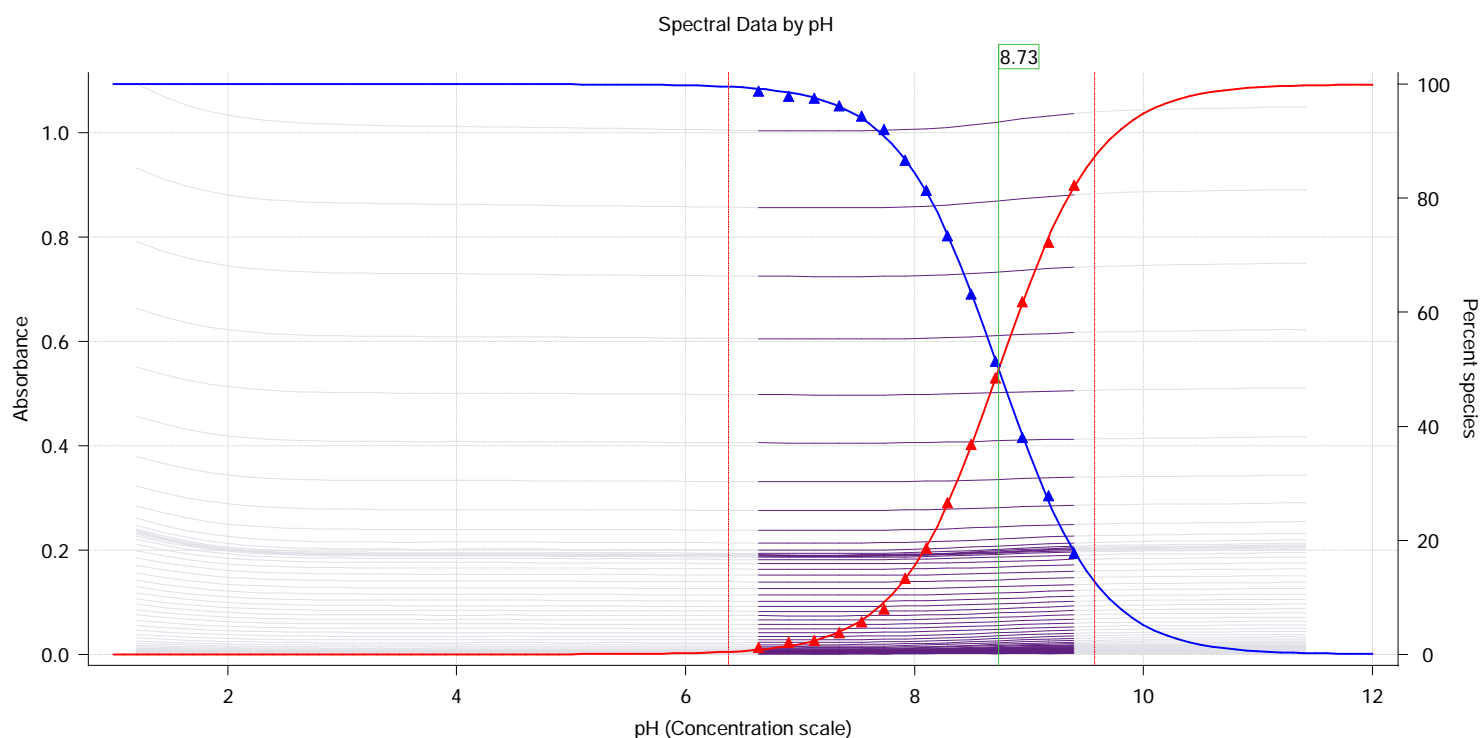
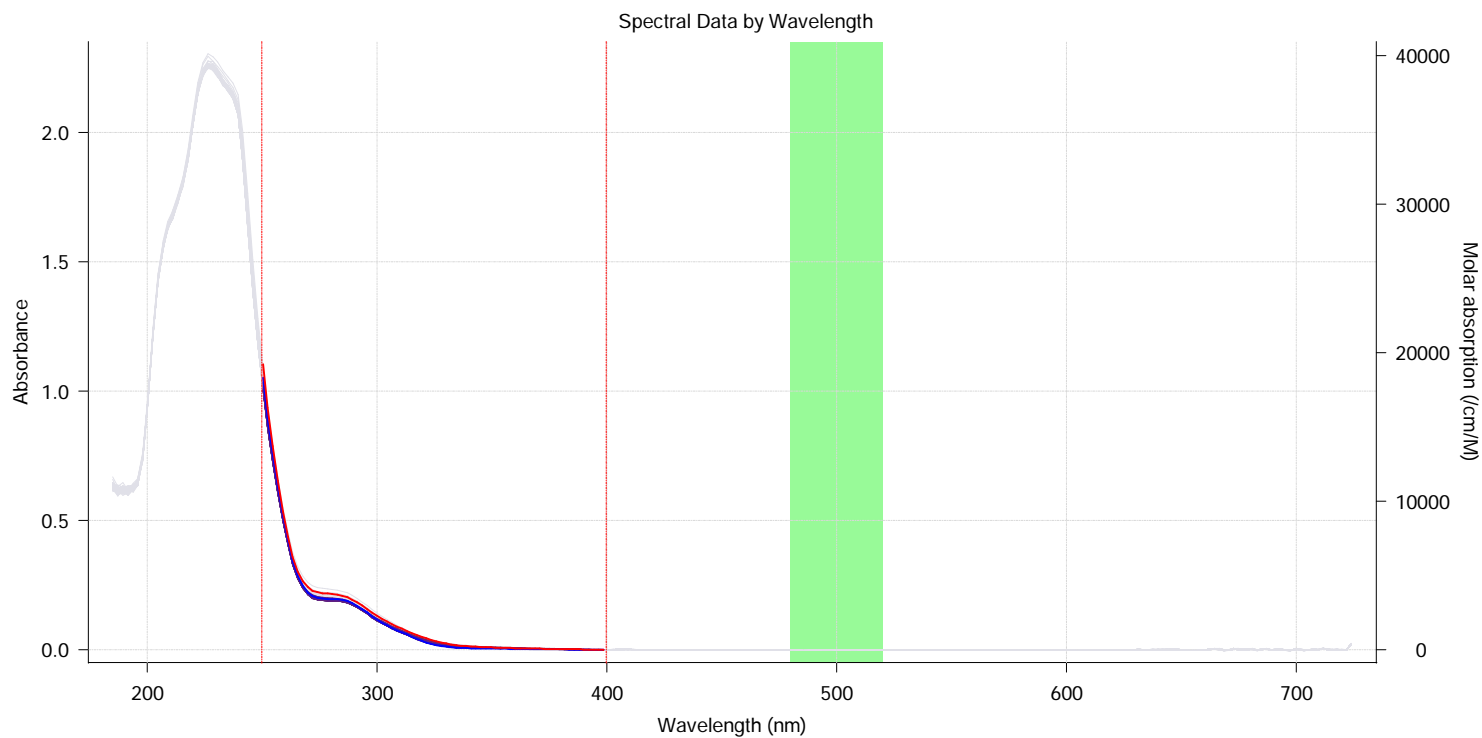


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Fast UV psKa Titration 2 of 3 11I-09014 Points 55 to 107

Graphs

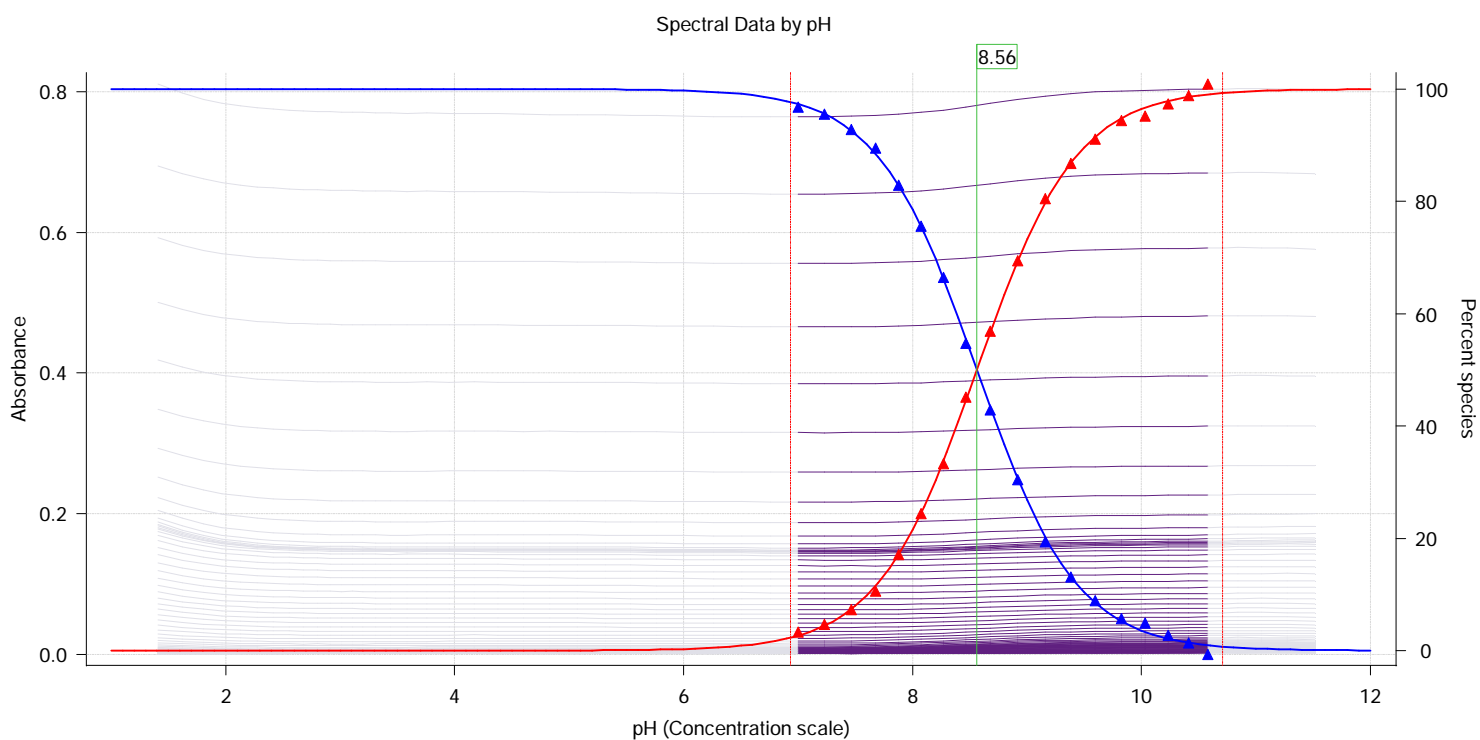
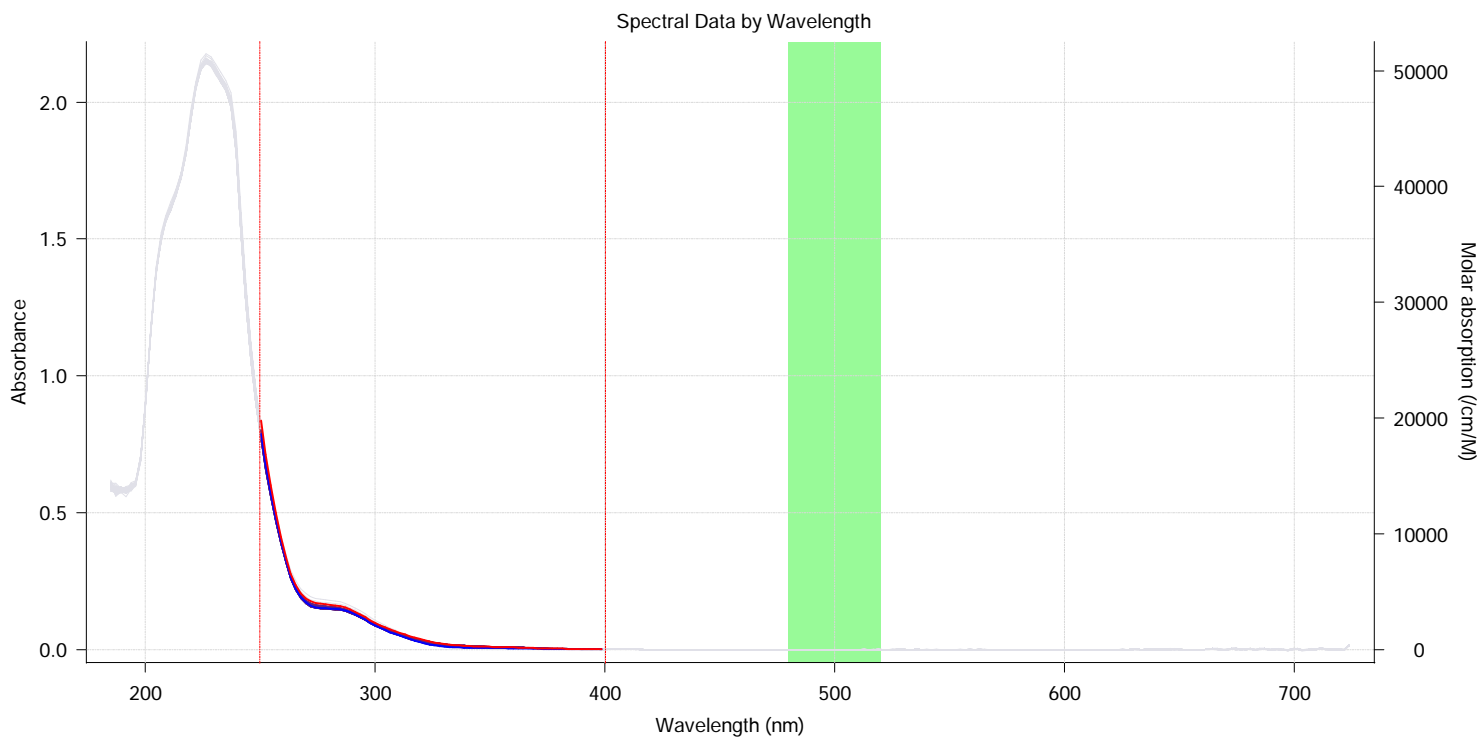


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Fast UV psKa Titration 3 of 3 11I-09014 Points 108 to 161

Graphs





Assay model

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Experiment start time: **09/09/2011 15:01:18**
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Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000275		
Sample by	Volume		
Sample volume	0.0150 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	09/09/2011 13:44:20	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Molecular weight	340.71		
Individual pKa ionic environments	No		
Number of pKas	1	09/09/2011 13:44:20	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Sample is a	Base	09/09/2011 13:44:20	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 1	4.00	09/09/2011 13:44:20	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logp (XH +)	-10.00	09/09/2011 13:44:20	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logP (neutral X)	-10.00	09/09/2011 13:44:20	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
